Visualization of Atomistic Simulation Data for Spatio-Temporal Information

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We have been developing an efficient scheme to support interactive visualization of the atomistic simulation data. Our scheme adopts two perspectives, which differ in their purposes and in how they process and render the data. First, to navigate through the data and to get an overall idea of spatio-temporal behavior of the system, the complete dataset is rendered using all-particle-display animation, all-particle pathlines and color-mapped-dimension representation techniques. Second, to gain a better understanding of the system for important local structural information, additional data, such as pair correlation functions, coordination numbers, are generated and rendered. Also, the clustrering techniques such as Minimum Spanning Tree (MST) and Nearest Neighbor Approach (NNA) are used to see how the system structure varies over time and what sort of structures are preserved. Finally for the categorization of the atoms according to their local environment, we used Common Neighbor Approach (CNA).

Automated Workflow for Generating Equations of State of Materials from First Principles

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Obtaining equation of state or elasticity at finite temperatures from first principles (FP) is a time consuming procedure that involves hundreds of job submissions and executions. Results from some runs must be used as parameters in the subsequent ones. This data flow between executions is usually prepared by the user. However, data manipulation between runs and decisions to be made during workflow executions are well defined. This permits workflows to be programmed and scheduled for automatic execution.

We present an algorithm/workflow for automatic equation of state and elasticity computations. Human involvement is restricted to the elaboration of a single initial input, which is not much more complex than the typical input for a single run of a FP code. Presently the algorithm makes extensive use of ***awk***, shell scripting, and three auxiliary C programs. The workflow exhibits high degree of parallelism and is well suited for implementation in distributed environments

Visualization in the Earth Sciences: A Discussion on Various Visualization Methods using amira®

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It is widely acknowledged that an important aspect in Earth Science research is the ability to visualize huge amounts of data resulting from numerical simulations or data acquisition. Whether the data is a simple two-dimensional plot or a three-dimensional multivariate grid, the ability to visualize the data is imperative for researchers to properly demonstrate results. This poster will examine various visualization techniques of the software package, amira® (www.amiravis.com) with respect to three research projects. These projects are: a mantle convection simulation run on the Earth Simulator; a spherical harmonic model computed at the University of Minnesota's Supercomputing Institute; an upper mantle study of earthquake-generated shear waves down to 660 km obtained through computed tomography using seismogram data from the Incorporated Research Institutions for Seismology (IRIS). The data resulting from the mantle convection study is in the form of a regular cartesian grid consisting of various field parameters such as temperature, velocity and viscosity. Techniques employed to view these fields include but are not limited to volume rendering, illuminated streamlines and oblique slices. The spherical harmonics model is rendered as a volume and is also explored using an isosurface module. The upper mantle study is visualized using an oblique slice technique and also isosurfaces. An analysis of the benefits and drawbacks of various amira® modules in regard to the above projects will not only result in a better understanding of the data, but will also demonstrate the unique capabilities of the different techniques and how they can be best applied to specific problems in the Earth Sciences.

Deep Melting of Carbonated Peridotite Beneath Oceanic Ridges

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Incipient volatile-assisted melting at 150-300 km may be required to explain geophysical anomalies beneath mid-ocean ridges and may have a profound influence on the geochemical cycling of heat producing (U, Th, and K) elements and rare gases, but experiments constraining the likely depth of melting of volatile-bearing peridotite similar to the natural mantle have been lacking. Experiments determining the solidus of carbonated peridotite from 3-10 GPa indicate incipient melting beneath ridges occurs at depths up to 300-330 km, producing 0.03 – 0.3 % carbonatite liquid. These melts may promote recrystallization and realignment of the mineral matrix, which may explain the geophysical observations. Extraction of incipient melts of carbonated peridotite deep beneath ridges may produce a vast mantle residue depleted in highly incompatible elements and fractionated in key parent-daughter elements.

Dynamic Web Services for Data Analysis in the Geosciences

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Current large-scale multidisciplinary efforts involve a combination of computation, visualization, and data analysis over geographically distributed environments. There is an urgent need to develop easy to use middleware systems that can dynamically adjust themselves to the needs of the researchers, while at the same time shielding them from the underlying details. In this poster, we present a framework that supports fault tolerance, collaboration, and the automatic linkage of web services selected by the user at runtime. We address this problem through a a unique and flexible middleware architecture (WEBIS), based on the NaradaBrokering (NB) middleware application program interface (API) (http://www.naradabrokering.org, [1]). NB is based on a publish/subscribe mechanism whereby all messages are sent to a system with a topic tag, to be received by any entity that has subscribed to that tag. This simple approach enables natural implementation of resource discovery, fault tolerance, system monitoring, and collaboration. On the server side, there is an increasing number of so-called web services available, ranging from weather services to sophisticated GIS (Geographic Information Services) systems that provide clients with querying capability. These services adhere to existing standards and are fully described through a WSDL (WebService Definition Language) file, many of which are publicly available. In this poster, we will demonstrate a proxy service whose role is to connect existing web services to our framework based on user requests. After selecting a desired web service from one or more registries, a user interface is created automatically based on the information contained in the WSDL file. This enables clients to interact with the service. This is illustrated through a service that computes the wavelet transform of three-dimensional scalar data files. The transformed data is processed by a second service that generates a bitmap (using the visualization software package Amira [2]) which is finally returned to one or more clients. Collaboration between two or more users are also demonstrated, along with fault tolerance. References

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HPSearch – Scripting Architecture for managing Distributed Components

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Scientific computing applications employ a varied number of data sources, data processing applications and visualization tools usually located over geographically distributed environments. There is a need to combine these geographically disparate services and link them together to form a complete application. Although this issue has been partially resolved using high performance messaging systems such as NaradaBrokering [NB], there is still an issue of deploying and managing the actual broker network and the application components.

The core issue of manageability of application components involves setting up various components (such as the virtual broker network) and linking various data sources, processing applications and visualization tools in a service oriented workflow. We have developed a scripting architecture to help manage some of the core issues. HPSearch [HPSearch] allows us to deploy the broker network topology and also modify it at runtime by creating links between brokers or deleting existing links. This is helpful in changing routing characteristics of the messaging substrate at runtime to improve performance. Further, HPSearch contains a container component, WSProxy, which helps to deploy quick data filtering and processing applications or wrap existing applications as Web Services. WSProxy also manages data input / output by mapping input and output data streams to NaradaBrokering topics. The overall application then can be setup and the execution of components may be orchestrated by using the HPSearch's scripting architecture.

We demonstrate the use of this application in GIS services by modeling the RDAHMM [RDAHMM] and Pattern Informatics applications. In each case we setup the broker network using the scripting interface. The next step is to initialize the components of our system (involves subscribing / publishing to correct topics and linking components together). The flow is then started by sending an appropriate message to the data source. As the data source publishes data onto the specified topic, this data stream is filtered by the data filtering service and resultant data is passed onto the data processing application. This stream may be formed from mined data from a data warehouse or could be directly from a sensor network. After processing, the data may be streamed out to the visualization service.

In addition, we leverage the use of a third party context service [CONTEXT] to maintain session and service information. This information is managed by HPSearch and allows correlating different instances of the same application.

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HPSearch	*HPSearch Project*, http://www.hpsearch.org
RDAHMM	*A Scripting based Architecture for Management of Streams and Services in Real-time Grid Applications* Harshawardhan Gadgil, Geoffrey Fox, Shrideep Pallickara, Marlon Pierce, Robert Granat In Proceedings of the IEEE/ACM Cluster Computing and Grid 2005 Conference, CCGrid 2005, Cardiff, UK
CONTEXT	Mehmet S. Aktas, Geoffrey Fox, Marlon Pierce *Managing Dynamic Metadata as Context* Istanbul International Computational Science and Engineering Conference (ICCSE2005) June 2005

Diamond-Cell Measurements of Fluid Viscosity and Activation Energy at High Pressures

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Significant advances in high pressure–temperature experiments now make it possible to measure the viscosity of fluids at deep-planetary conditions. This is important because viscosity is often the rate-limiting factor for internal planetary dynamics, yet it is poorly understood from a theoretical perspective.

New rolling-sphere measurements on methanol and a 4:1 methanol:ethanol mixture, using a resistance-heated diamond-cell, yield an activation energy of 18 to 98 kJ/mol over the pressure–temperature range of 0-6.5 GPa and 298-338 K. These alcohols are potential analogs for structured liquids, such as the silicate melts of the Earth's interior, and are also important as pressure-transmitting media in diamond-cell experiments. Our data are in good agreement with previous measurements at room temperature, and we find that activated-state (Arrhenius), free-volume, and power-law models fit the data within our uncertainties. Extrapolation based on these models yields glass-transition pressures (10^{12} Pa s) below 11 GPa at room temperature. As our measurements extend beyond the equilibrium crystallization pressure of methanol, 3.6 GPa at 300 K, they provide information about viscous relaxation of the metastable liquid state.

The rolling-sphere technique can be applied to liquid metals in the diamond cell by using synchrotron radiation to obtain x-ray shadowgraphs. In-situ measurements can be made by placing materials with different x-ray absorption in a liquid metal in order to determine viscosity either (or both) by rolling-sphere or Brownian-motion measurements.

Finite Prandtl Convection

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Convection in fluids with Prandtl numbers of order 10^4 is important in a wide variety of planetary situations such as the partially molten ice plumes of Europa or the magma oceans of early planetary interiors. Convection in fluids with Prandtl numbers above 10^3, have previously been modeled numerically using the infinite Prandtl approximation. This is the same approximation used for the Earth's mantle, which has a Prandtl number of 10^{25}. It was assumed that by Prandtl numbers of order 10^3, the inertial terms no longer contributed significantly towards the convection behavior. This assumption, however, had not been previously tested numerically due to the fact that the inertial terms in the finite Prandtl equations become very stiff as Prandtl number increases requiring increasing grid sizes. We conducted studies of 2-D plumes with Prandtl numbers up 2×10^4. We found that these plumes tend to be hotter and to grow much faster than those modeled using the infinite Prandtl approximation.

In collaboration with Alain P. Vincent and David A. Yuen

The predictability of finite Prandtl Convection

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We have used four-dimensional variation assimilation along with the adjoint equations of finite Prandtl convection to study the predictability of these types of systems. We found that the adjoint method is very powerful correcting simulations with unknown initial conditions but for which data, such as heat fluxes over time, was available during the simulation run. This method could be used to better constrain numerical simulations with laboratory data or to study convection backwards in time in planetary bodies for which heat flux or other observations are available. The time for which the system can be predicted, however, decreases with increasing Rayleigh number and decreasing Prandtl number.

Constraining the Internal Composition and Thermal State of Mars

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The existence of a Martian core has been widely accepted for some time now and even more so now given its ability to explain in a natural way the presence of the strong, spatially variable magnetic fields found by the MGS spacecraft. An ancient internal dynamo in analogy to the Earth is assumed to have been present which has magnetised the crustal material as it cooled through the Curie temperature. Other supporting evidence for a core comes from the SNC meteorites. These are found to be highly depleted in siderophile elements which, like on Earth, is attributed to their removal during core formation. The mean moment of inertia in combination with the mean Martian density can give us an idea of the size of the core, as we do not know its composition nor that of the mantle. However, compositions of Martian meteorites in combination with models of the planet's radial density distribution inferred from geophysical constraints, like mass and moment of inertia, lead to inferences about the composition of the Martian mantle. From this the size of the core is generally believed to be around 1300-1500 km in radius. Presently we are attempting to invert these geophysical data to obtain information on the internal composition and thermal state of Mars using a Gibbs free energy minimisation routine to calculate the stable phases present. The data used in the inversion are, mean moment of inertia (I/MR^2), mean density, second degree tidal Love number (k2), tidal dissipation factor and of course mean radius (R). Their values are, in the above order, 0.3649Â±0.0017, 3933Â±0.4 kg/m3, 0.145Â±0.017, 92Â±11 and 3389.5 km, respectively.

High pressure studies on cadmium oxide and zinc oxide: From first principles calculations to experiments

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Modern computational science has reached a level of accuracy where the theoretical calculations could be used for establishing the "true" behavior of perfect materials, whether materials are realized in nature or not. However, accurate experimental data are still, and will be, the primary standards toward the testing or benchmarking of calculations and simulations. *In situ* high-pressure x-ray diffraction experiments were performed up to 176 GPa for CdO, and phase transitions from NaCl- to CsCl-type structure were found around 90 GPa, which is in good agreement with density functional theory total energy calculations. Improvement of the theoretical calculation is expected for the 4*d* and 3*d* transition-metal monoxides CdO and ZnO if these ultrahigh pressure experimental data of the bulk modulus and lattice constant of the *B*2 phase of CdO could be used as input to the calculations.

The pressure induced phase transition for ZnO from wurtzite-to-rocksalt structure around 9 GPa was first reported in 1962. The mechanism responsible for this pressure induced phase transition, however, is not yet fully understood. Very recently, two separate groups reported the results of first-principles calculations on the possible path that would allow the least costly crossing of the transition enthalpy barrier. From these calculations, the existences of possible metastable structures, i.e., an intermediate "tetragonal" phase, or "hexagonal" phase, were proposed, respectively. The pressure dependence of structural parameter *u* of wurtzite phase ZnO in helium pressure medium at room temperature was studied by Rietveld refinement of high resolution angular dispersive x-ray diffraction. The distortion by hydrostatic pressure with pretransitional effect demonstrates that the initial intermediate distortion path prefers the hexagonal model. These structural evolutions under pressure derived from refinement provide experimental confirmation to the corresponding first-principles simulations.

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High pressure behavior of hydrous phases

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We explore the structure and physical properties of brucite over a wide range of pressures with density functional theory using the variable cell shape plane wave pseudopotential method in the local density (LDA) and generalized gradient (GGA) approximations. We probe the energetics underlying the structure and dynamics of the proton sub-lattice by performing a series of constrained and unconstrained static calculations based on an energetically stable sqrt(3)x sqrt(3)x 1 super-cell wherein proton locations are related to the 6i Wyckoff sites as opposed to the ideal 2d site. The displacement of the hydrogen from the 3-fold axis increases with increasing pressure. This means that even in the absence of thermal energy, the protons are frustrated and would be expected to exhibit long-range disorder akin to a spin glass. In order to shed light on the dynamic nature of the proton hopping between the 6i-like sites, we have determined the activation energy barrier for such jumps. We find that the energy barrier increases with compression, possibly indicating a transition from dynamic proton disorder at lower pressures to static disorder at higher pressure. We have also investigated the possibility of proton jumps across the interlayer, by determining the potential energy well along the O...O vector. We infer that proton jumps across the interlayer are either severely limited or highly cooperative since we do not find any evidence of a double well along the O...O vector. The absence of a double well along the O...O vector, the evolution of O-H...O distances with compression and the gradual transition to a symmetric O-H...O configuration, all argue for weak hydrogen bonding in brucite.

In collaboration with Lars Stixrude

Deformation response of (n 1 0) symmetric grain boundaries in rocksalt-structured materials

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There have been substantial advances in the study of plasticity in minerals at high pressures in recent years. However, a complete understanding of the role of microstructure in these deformation processes is still lacking. Here we present the results of some recent atomistic simulations dealing with symmetric (n 1 0) tilt grain boundaries in rocksalt-structured minerals subjected to various simple loading conditions. These simulations have elucidated the atomic mechanisms active in a number of processes, including a pressure induced rearrangement in these grain boundaries that may have broad implications for diffusional and dislocation modes of deformation in minerals at high pressures. A remarkable reduction in sliding resistance of the (n 1 0) grain boundaries accompanies this transformation in rocksalt-structured materials. We present atomic and continuum models that account for the boundaries' relative stability and mobility.

The Local Properties of a Fe Impurity in MgO

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The existence of a high spin to low spin transition of Fe in lower mantle minerals would have implications for geological phenomena, such as, Fe enrichment in the lower mantle and the scale of mantle convection*. With the GGA approximation of density functional theory, we calculate the electronic structure and vibrational spectrum of a 3x3x3 MgO cluster with Fe substitution at the center site. We describe the influence of the Fe impurity on the vibrational modes and the pressure dependence of the crystal field splitting and Hund splitting of the Fe d-orbitals.

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In collaboration with Phil Allen

The Effect of Large Melt Fraction on the Deformation Behavior of Peridotite

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We have performed a series of high-temperature, triaxial compressive creep experiments on dry, synthetic peridotites in a gas-medium apparatus at a confining pressure of 300 MPa and temperatures from 1498 to 1556 K in order to determine the influence of large amounts of melt ($0.15 < \varphi < 0.30$) on the rheological behavior of partially molten rocks in both the diffusion and dislocation creep regimes. Our samples consisted of mechanical mixtures of crushed and dried San Carlos olivine (10 or 50 μm) plus MORB (~8 μm) that we isostatically hot-pressed at 1523 K and 300 MPa for 4 to 10 h. After hot-pressing, the melt is homogeneously distributed between grain-size melt pockets at triple junctions and smaller pockets at two-, three- and four-grain junctions. Stress versus strain rate data from samples containing $\varphi = 0.15$ to 0.30 MORB with a grain size $d \approx 10$ and 50 μm deformed at 1500 to 1553 K and differential stresses of 1 to 180 MPa reveal a drop in rock viscosity of several order of magnitude between $0.25 < \varphi < 0.30$ that is independent of strain rate over the range 10^{-2} to 10^{-6} s^{-1}, indicative of the rheologically critical melt fraction (RCMF). In all of these experiments, we observed only a small amount of grain growth. Stress versus strain rate data from our creep experiments indicates that the flow behavior in both the diffusion and grain size sensitive dislocation creep regimes as well as the transition from diffusion to dislocation creep over $0 < \varphi < 0.25$ is well described by the published flow laws for partially molten samples of olivine + MORB deformed under anhydrous conditions (*Hirth & Kohlstedt*, 2003) with $\varepsilon \propto \exp(\alpha\varphi)$ and $\alpha = 21$ for diffusion creep (Newtonian) and $\alpha = 32$ for grain boundary sliding (GBS) accommodated by dislocation creep.

Infrared and thermal transport properties of MgO

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The transmission and reflection infrared spectra of single crystal MgO are measured experimentally. The dielectric constant, absorption coefficient are fitted with classical oscillator model. The spectra are also calculated using the empirical shell model and compared with experimental data. In the end, both vibrational and radiative thermal conductivity of MgO are calculated with shell model.

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In collaboration with Phil Allen

Amorphization and other anomalies in ice VIII under decompression

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Ice VIII is a prototypical form of high pressure ice expected to be abundant in icy planets' and satellites' interiors. Experimentally it has been known that under decompression ice VIII exhibits anomalous behavior outside its stability field: strong nonlinear pressure dependence of phonon frequencies and structural parameters and eventually amorphization upon heating. Our GGA calculations find phonon collapse at a slightly negative pressure, corresponding to amorphization with increasing temperature. The nonlinear behavior of phonon frequencies is well reproduced and found to be a precursor to amorphization, not a sign of an isosymmetrical phase transition as previously proposed. Within our accuracy there is no indication whatsoever of such subtle phase transition.

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Phase transitions in ice studied by first principles

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Ice has an intricate phase diagram. Up to now, thirteen crystalline phases have been identified experimentally. They can be grouped into two classes: phases of a single hydrogen-bond network (1HBN) with low density and those of two interpenetrating networks (2HBN) with high density. In ice XI, a prototypical form of 1HBN ice, our GGA calculation shows a pressure-induced an incommensurate phonon instability is followed by a collapse of the acoustic branch, predicting instabilisties in all lengths scales, which we interpret as pressure-induced amorphization. "Static" compression bypasses amorphization and shows a continuous relationship between 1HBN and 2HBN structures. This suggests that amorphization occurs as along the transformation path between two radically distinct structures, 1HBN and 2HB. We also investigate the order-disorder transition in ice VII-VIII, two prototypical forms of 2HBN ice. The disordered phase is addressed through a complete statistical sampling of molecular orientations of a 16 molecules supercell. We reproduce quite well the experimental phase boundary, in contrast with previous force field calculations that could not reproduce even the Clapeyron slope sign.

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Post-perovskite transition in $NaMgF_3$

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We have investigated through first principles computations the pressure-induced behavior of $NaMgF_3$. It has the same *Pbnm* perovskite structure as $MgSiO_3$, the major lower mantle phase. Likewise $MgSiO_3$ it displays the same post-perovskite transition. Static LDA calculations indicate this transition should occur shortly after 17.5 GPa and the latter decompose into NaF and MgF_2 at 40 GPa. These phases are shown to be mechanically stable. The existence of a post-perovskite transition at low pressures in this material makes possible studies of properties of such phase more easily accessible in a lower pressure range by various sorts of experiments.

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VLAB and the Earth

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Our knowledge of the state and processes of the Earth's interior is tied to the physical and chemical properties of the constituent materials at the local pressure and temperature. Seismology provides *in situ* measurements of the acoustic velocities. Lateral and radial variations in velocity can be converted to chemical and/or thermal variations only if we know the effects of chemistry and temperature on these properties. Driving forces for convection must be obtained through the relationship between velocity perturbation and density. Atom diffusion controls the rate that plates can overturn. Pressure induced phase transformations dominate the radial seismic signal.

Recent convergence of experiment and theory offers new challenges for calculating these important properties. We must continue to ground truth the theory with experiments and use theory to explore those regions of P – T space that are inaccessible with experiments.

The QUANTUM-ESPRESSO **Project**

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QUANTUM-ESPRESSO is a collaborative, open-source project [1] for quantum-mechanical simulations of extended or isolated systems based on density-functional theory, periodic-boundary conditions, plane-waves, and norm-conserving or ultrasoft pseudopotentials. QUANTUM-ESPRESSO integrates in a new, modular and multi-platform framework the electronic-structure packages developed in the last two decades by groups in Trieste [2] and in Lausanne [3], and rewritten for this project. The QUANTUM-ESPRESSO core is based on the self-consistent determination of ground-state energies and forces, Car-Parrinello molecular dynamics, and linear-response theory, implemented in a fast and scalable architecture that includes extensive use of libraries (BLAS, LAPACK, MKL, FFTW), optimal parallelization over plane-waves, FFT grids, and k-point meshes, and (CP only) a very efficient implementation of Gamma-sampling and ultrasoft box-grids. Advanced capabilities include the calculation of phonon eigenvalues and eigenvectors, effective charges and dielectric constants, Berry-phase polarization, electron-phonon coupling and phonon lifetimes, infrared and Raman cross sections, spin-orbit coupling and non-collinear magnetism, electric field gradients, nudged elastic-band methods and string dynamics, ensemble density-functional theory, maximally-localized Wannier functions, and molecular dynamics in the microcanonical, canonical, isoenthalpic, and isoelectric ensembles. Input via the graphical user interface PWgui is integrated into the package, and visualization performed via the public-domain XCrysDen package (`http://www.xcrysden.org`).

QUANTUM-ESPRESSO stands for *Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimisation*; its development is led by the Italian National Simulation Center DEMOCRITOS (hosted by the International School of Advanced Study in Trieste), in collaboration with ICTP Trieste, CINECA Bologna, Scuola Normale Superiore in Pisa, Princeton University, MIT, and all their respective funding agencies. The package and its tutorials are distributed under the GNU General Public License and made available to the scientific community worldwide at `http://www.quantum-espresso.org`. Electronic-structure schools and classes based on this software are periodically offered in developed and developing countries, with additional support from the UNESCO/IAEA International Center of Theoretical Physics in Trieste.

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